Supplementary Information

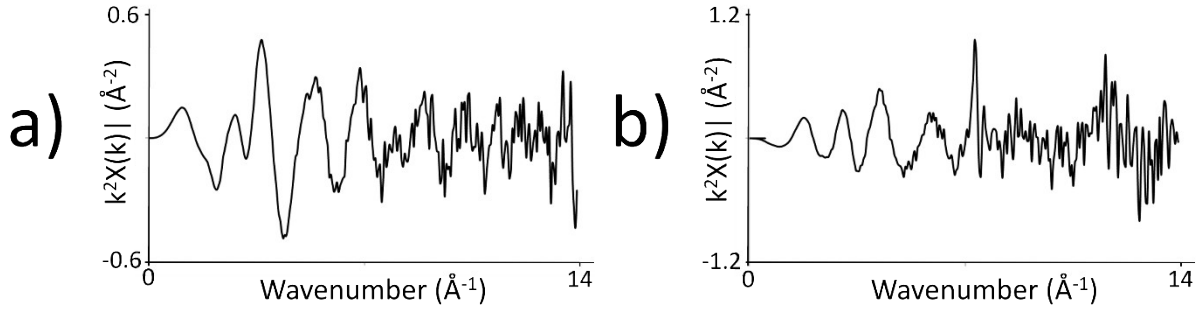

Fig. S1 k-space (k^2-weighted) for the a) Au L_3-edge and b) Ag K-edge of $Au_{104}Ag_{40}$.

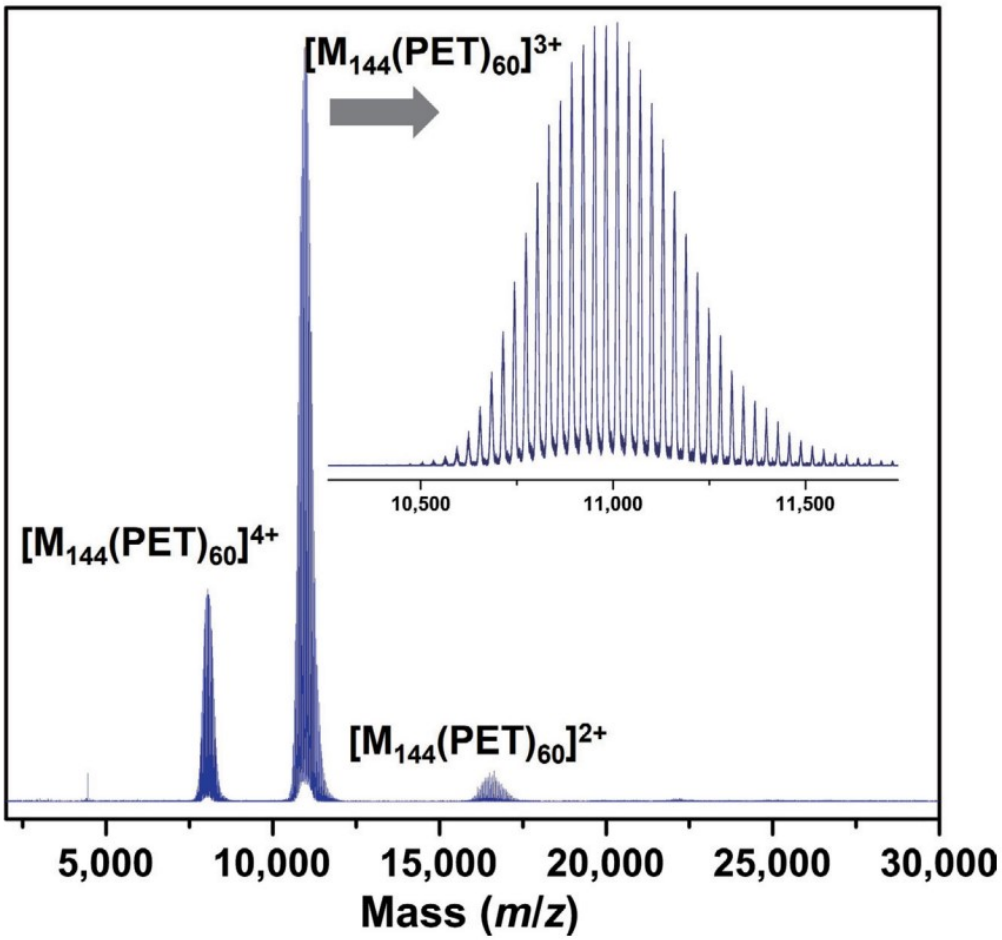

Fig. S2 Previously reported[30] ESI-MS spectrum of $Au_{104}Ag_{40}$. Inset shows zoomed in view of 3+ peak set.

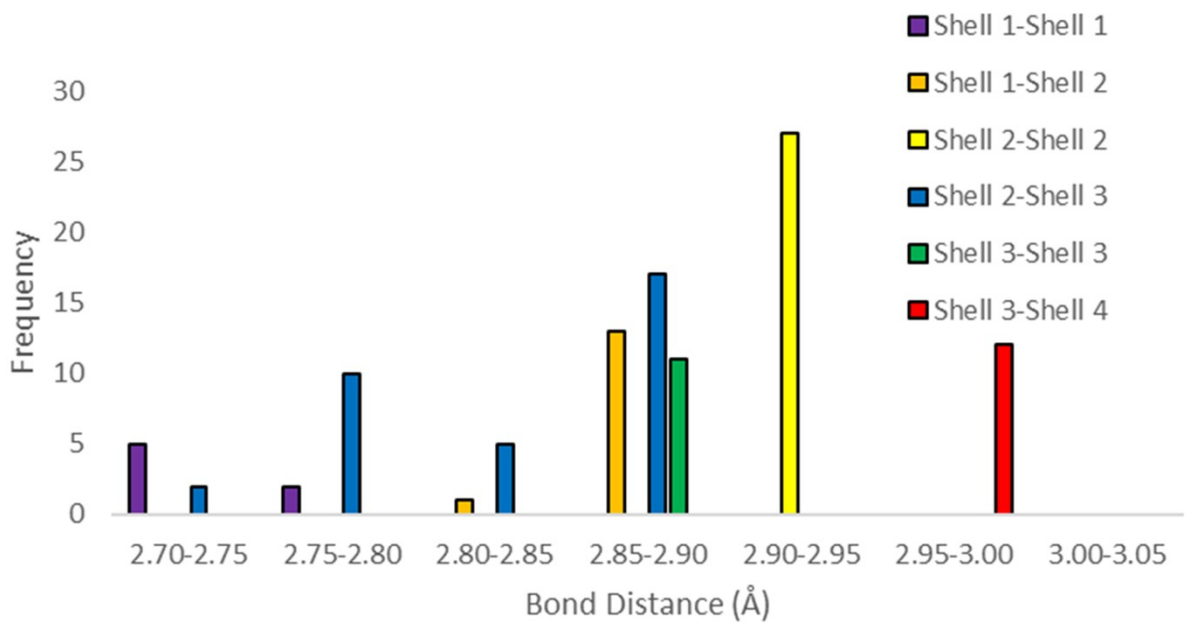

Fig. S3 Bond distribution for the Au_{144} NC. General trend is that bonds between atoms towards the core of the NC are shorter in length, and bonds between atoms towards the surface of the NC are longer in length. This information can aid in the assignment of Ag dopant locations in $Au_{104}Ag_{40}$ through comaprison of bond distances determined through EXAFS fitting.

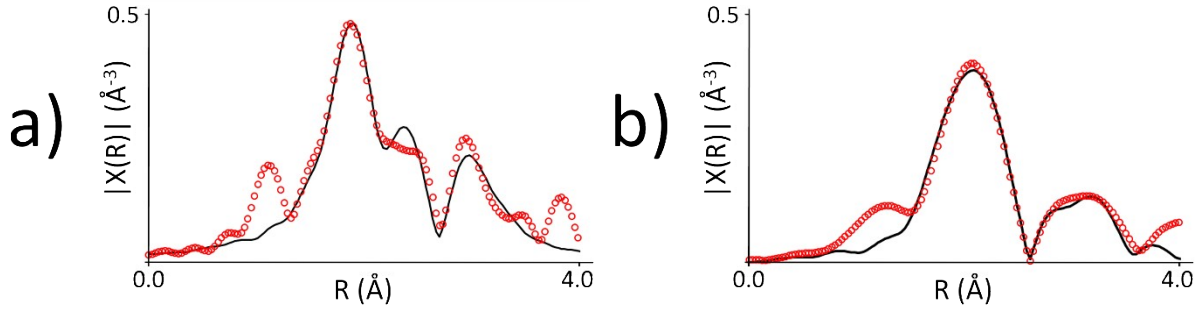

Fig. S4 Fitted FT-EXAFS spectra for the a) Au L_3-edge and b) Ag K-edge of $Au_{104}Ag_{40}$. Peaks arise from bonding interactions within the sample. Intense peak ~2.0 Å in each spectra is characteristic of a M-S bonding interaction. Doublet peak in the Au L_3-edge spectra ~2.5-3.0 Å is characteristic of Au-M alloy interactions. Peak in the Ag K-edge spectra ~3.0 Å is characteristic of Ag-M alloy interactions. The relative intesnity of each peak also provides insight into the CN of each interaction. Au-S and Ag-S CNs are roughly equal, while the Au-M CN is expected to be higher than the Ag-M CN.

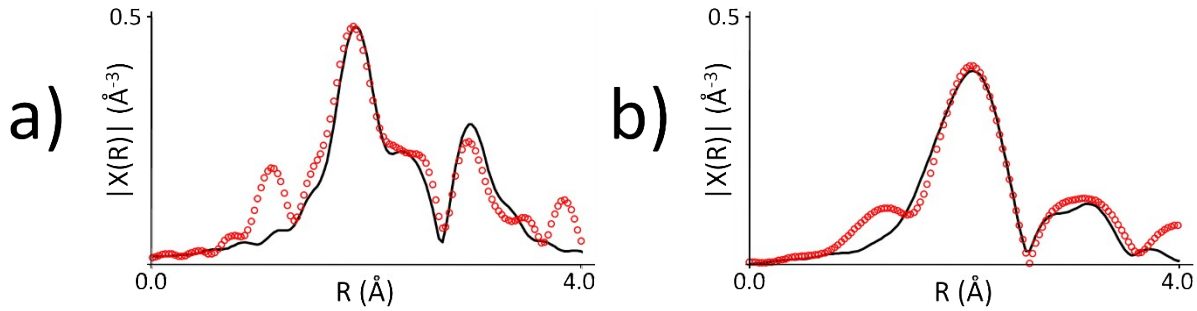

Fig. S5 Fitted FT-EXAFS spectra for the refined fit of the a) Au L_3-edge and b) Ag K-edge of $Au_{104}Ag_{40}$. Fit quality is slightly improved upon fixing the CN according to values from the proposed model, providing evidence of its accuracy.